Application Serial No. 09/506,717
Amendment dated October 28, 2004
Reply to Office Action dated May 28, 2004

REMARKS

By the present Amendment, claims 5, 9, 10, 12, 16, 20, and 21 have been amended. No claims have been added or canceled. Accordingly claims 5-16 and 19-21 remain pending in the application. Claims 5, 9, 10, 12, 20, and 21 are independent.

In the Office Action of May 28, 2004, claims 11, 13, 14, and 16 were rejected under 35 U.S.C. §112, first paragraph as failing to comply with the written description requirement. Claims 10 and 16 were rejected under 35 U.S.C. §112, second paragraph as being indefinite for failing to particularly point out and distinctly claim the subject matter regarded as the invention. Claims 5-16 and 19-21 were rejected under 35 U.S.C. §101 as being directed to non-statutory subject matter. Claims 5, 11, 15, and 20 were rejected under 35 U.S.C. §102(b) as being anticipated by Graovac et al. [JACS 95(19):6267-6273 (1973)]. These rejections are respectfully traversed.

Rejection under 35 U.S.C. §101

Claims 11, 13, 14, and 16 were rejected under 35 U.S.C. §112, first paragraph as failing to comply with the written description requirement. Specifically, the Office Action alleges that these claims contain subject matter which was not described in the specification in such a way as to reasonably convey to one skilled in the art that the inventors had possession of the claimed invention at the time the application was filed.

At the outset, Applicant would like to point out some inconsistencies regarding the Examiner's position on this rejection, as well as the overall timeliness. In the Office Action dated 6/17/02, the Examiner withdrew the rejections under 35 U.S.C. §112, first paragraph. In

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the subsequent Office Action (dated 4/23/03), the Examiner indicated claims 5, 9, 10, and 12-14

allowable. In response, Applicant amended the allowable claims, in part, to further prosecution

of this application. In the Office Action dated 10/23/03, the Examiner reinstated the rejection

under 35 U.S.C. §101.

With respect to claim 11, the Office Action alleges that the limitation of "queuing at least

a subset of candidates by priority" is not supported by the specification. The Office Action

further indicates that the specification only supports priority queuing of ESVDs "leftover after

the best possible ESVDs have been pursued. Alternatively, the Office Action indicates that only

inferior ESVDs are queued after the best ESVDs have been separately analyzed. The Office

Action alleges that the subset of ESVDs does not limit the subset to either leftover or inferior

ESVDs.

Applicant respectfully disagrees with the Examiner's conclusion. The specification does

not require that the subset of ESVDs be limited to leftover or inferior ESVDs. The Examiner

correctly identifies one exemplary embodiment which discusses leftover or inferior ESVDs. The

Examiner is attempting to limit the claims to one specific embodiment that is described in the

specification. However, nowhere in the specification is it stated that priority queuing requires

that the subset of ESVDs be limited to leftover or inferior ESVDs. The claims should not be

limited only to embodiments specifically described in the specification, which is intended to be

illustrative and not limiting. Otherwise, every conceivable embodiment would have to be

described in the specification. Further, the M.P.E.P states that "[t]he subject matter of the claim

need not be described literally (i.e., using the same terms or in haec verba) in order for the

disclosure to satisfy the description requirement." See M.P.E.P §2163.02.

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      Applicant further submits that the specification is replete with examples of evaluative

actions, including examples indicated by the terms underlined in the following excerpts of the

specification at pp. 5-10:

>   Conceptually, in a specific embodiment of the procedure, a path is
> traced through the structure and, for each atom, each possible electronic
> and bonding state <u>is examined that is consistent with previous results</u>
> along the path. By <u>extensively or exhaustively examining possible states</u>
> <u>and orders</u>, the procedure is able to arrive at a fixed bond solution, if one
> exists.
>
>   ...
>
>   <u>All possible ESVDs may be attempted for all atoms</u>, and all bond
> orders (including single and double) may be attempted for all bonds. <u>A</u>
> <u>solution is determined to have been found when</u> a combination of codes
> and orders is self-consistent, such that, for every atom, the orders of bonds
> to the atom match the requirements of the atom's ESVD, and the net
> charge and number of paired electrons of the system are also as required
> by the structure. Possible further requirements include a <u>satisfactory</u> 4n+2
> electron count or an absence of radicals or zwitterions.
>
>   In a specific implementation, the procedure includes several
> practical features that help to produce timely results in practice. A first of
> the practical features reflects a recognition that it is not always necessary
> to try all ESVDs and bond orders: with respect to choosing an order for a
> bond to an atom having an assigned ESVD, <u>the only orders considered are</u>
> <u>orders that are consistent with the ESVD</u>, taking account of bonds already
> assigned. For example, if a carbon ([121/1]) has been assigned a double
> bond, the carbon's next bond may not be double, and is only considered to
> be single. Further, <u>the only ESVDs that are chosen</u> are ESVDs that are
> consistent with adjacent fixed bonds.
>
>   A second of the practical features is consistent with a recognition
> that in practice many or most solutions do not involve unpaired electrons
> or charge: <u>ESVDs featuring unpaired electrons or charge are not</u>
> <u>considered initially. If a solution is found without referring to such</u>
> <u>ESVDs</u>, the procedure is finished, and time has been saved.
>
>   According to a third of the practical features, the procedure is only
> partially recursive. With respect to bond orders, when alternative bond
> orders are attempted, recursion is sensible: if a single bond appears to be
> the most advantageous next step, and <u>its recursive development returns in</u>

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failure, the double bond remains the most advantageous next option. In
other words, pursuit of a bond order is exhaustive. By contrast, with
respect to ESVDs, some ESVDs tend to be more promising (i.e., better)
than others, in at least some cases. Accordingly, after the possible ESVDs
for an atom are tabulated, the best of the possible ESVDs is actually
pursued, recursively, and the rest of the possible ESVDs are placed in a
priority queue, keyed to a rating of the inchoate structure's likelihood of
success. In this way, less promising ESVDs are not examined until more
promising combinations are exhaustively considered.

Another of the practical features in a computer-based
implementation is an implementational measure that speeds the
assessment of compatibility between bonds and ESVDs: a screening
bitmask. (A bitset is a piece of data, e.g., an integer, in which each bit
represents a Boolean value. As used herein, a bitmask is synonymous
with a bitset.) For a given ESVD, a screening bitmask encodes the
ESVD's bonding and electron requirements. Similarly, for an atom,
another screening bitmask specifies which types of bond have already
been fixed. When the latter screening bitmask is logically (i.e., bitwise)
subtracted from the former screening bitmask, a list of bond types still
required at the atom is obtained. By logically subtracting the former
screening bitmask from the latter screening bitmask, it can be determined
whether it is possible to apply the ESVD to the atom. Such operations
tend to save time, since multiple logical comparisons are compressed into
one comparison of bitmasks.

In a specific implementation, the screening bitmask for the ESVD
[121], for example, can be figured from Table 3 (Fig. 11). Only the
bonding portion of the bitmask is considered when choosing the bond
orders compatible with an ESVD. The internal single bond, the internal
double bond, and the external single bond of the ESVD [121] correspond
to bits #0, #2, and #4, respectively. Therefore, the bitmask has the value
{0,2,4}. For an atom that has had one single bond fixed, the bitmask
consists of bit #0, with the value {0}. The difference between the former
and latter bitmasks, {0,2,4} - {0} = {2,4}, reveals the fixed bond types
that must eventually be assigned to the atom, namely, an internal double
bond (bit #2 and an external single bond (bit #4).

An example of the opposite process is determining whether an
ESVD, such as [111/2-], is compatible with an atom that, for example, has
two fixed single bonds and which, due to a global restraint, may not be
charged. The ESVD's bitmask is {0,1,4,10,12,14}, indicating that the
ESVD has an internal single bond, has two internal single bonds, has an
external bond, is negative, is not positive, and does not have an unpaired

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> electron, respectively. The atom's bitmask is {0,1,8,11,12}, indicating the
> atom has an internal single bond, has two internal single bonds, is neutral,
> is not an anion, and is not a cation, respectively. The atom's bitmask
> {0,1,8,11,12} is not a subset of the ESVD's bitmask {0,1,4,10,12,14},
> which indicates that the ESVD is not compatible with the atom. Although
> the bonding portions are compatible, the electronic portions are not. (In
> general, the more fully characterized or developed an atom is, the more
> bits are set in its bitmask, and the less likely that the atom will be
> compatible with a given ESVD.)

Other evaluative action is described elsewhere in the specification, including in examples

described in the specification at pp. 11 et seq.

Applicant respectfully submits that the rejection of claim 11 under 35 U.S.C. §112, first

paragraph, should be withdrawn.

The Office Action Alleges that claims 13 and 14 provide a table that is "configured to

allow additional elements, etc. to be added", and that such a configuration is not found in the

application as filed. The Office Action further states that the disclosure does not show a table

which is specifically configured to allow additional elements. In response to Applicant's

arguments, it is indicated that the knowledge of one skilled in the art is not persuasive for such a

written description requirement.

Applicant again disagrees with the Examiner's conclusions regarding claims 13 and 14.

First, the claims of the application should be viewed in light of the understandings of one skilled

in the art. A skilled artisan would not interpret the table recited in claims 13 and 14 (and

described in the disclosure) as limited to the exact size shown in the figure. As set forth in the

M.P.E.P §2163.06, "[T]he Patent Act and this court's case law require only sufficient description

to show one skilled in the ... art that the inventor possessed the claimed invention at the time of

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filing." Citing *Union Oil of Cal. v. Atlantic Richfield Co.*, 208 F.3d 989, 997, 54 USPQ2d 1227-33 (Fed. Cir. 2000).

It is well known and accepted that tables used to store information are dynamically configurable to accommodate the addition and removal of entries. Applicant further directs attention to Figure 7 which explicitly specifies that the illustrated table shows <u>selected</u> electronic state/valence distributions. Additionally, the corresponding description indicates that the table "<u>is not a complete list</u>,..." See page 7, lines 5-6. Accordingly, a skilled artisan would readily recognize and appreciate that additional (i.e., elements and values) could be added. Further, the disclosure is intended to be illustrative, and not limiting. There is <u>absolutely nothing</u> in the disclosure to indicate that additional elements cannot be added to the table. The Examiner's suggestion that the claims cannot further define inclusion of additional entries is contrary to the specific disclosure that is found in the application. Further, the Examiner has not indicated exactly why someone would read the specification and conclude that additional properties could not be added to the table.

Applicant therefore respectfully submits that claims 13 and 14 are in full compliance with the requirements of 35 U.S.C. §112, first paragraph.

Regarding claim 16, the Office Action indicates that there is no indication of where the instant disclosure provides written support for "neutral, non-radical" representation of chemical structures. Accordingly, Applicant directs attention to page 11, lines 5-11; page 27, lines 6-17, and Figure 29.

Applicant therefore respectfully submit that independent claim 16 is in full compliance with the requirements of 35 U.S.C. §112, first paragraph.

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Claims 10 and 16 were rejected under 35 U.S.C. §112, second paragraph, as being

indefinite for failing to particularly point out and distinctly claim the subject matter regarded as

the invention. The Office Action cites several instances of language that is considered indefinite

or otherwise confusing.

Applicant has therefore amended claims 10 and 16 to address the issues of indefiniteness

raised in the Office Action.

It is respectfully submitted that claims 10 and 16 now satisfy the requirements of 35

U.S.C. §112, second paragraph. Withdrawal of this rejection is requested.

Rejection under 35 U.S.C. §101

Claims 5-16 and 19-21 were rejected under 35 U.S.C. §101 as being directed to non-

statutory subject matter. The Examiner states that the instant claims do not require performance

of a result outside of a computer. The Examiner states that the claims merely manipulate

chemical bonding structure information without any physical transformation outside of a

computer. The Examiner had also previously suggested that outputting the information outside

the computer may overcome such a rejection.

Applicant has reviewed the claims and made appropriate amendments to claims 5, 9, 10,

12, 20, and 21. Some of these claims now recite a further step of, for example, "outputting the

fixed bond information."

It is therefore respectfully submitted that claims 5-16 and 19-21 now satisfy the

requirements of 35 U.S.C. §101.

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Rejection under 35 U.S.C. §102(b)

Claims 5, 11, 15, and 20 were rejected under 35 U.S.C. §102(b) as being anticipated by

Graovac et al. [JACS 95(19):6267-6273 (1973)]. The Office Action alleges that Graovac

analyzes more than fixed bond information because non-fixed bond representations are depicted

in Figures 1 and 2. The Office Action indicates that there is no disclosed definition of what is

meant by "delocalized structure representation" that would distinguish over the representations

of Figures 1 and 2 in the reference. Accordingly, it is asserted that such delocalized structures

include chemical structures without localized bonds. The Office Action further asserts that Table

I of Graovac discloses the claimed priority queuing.

Applicant respectfully disagrees. Independent claim 5 defines a method for use in

deriving fixed bond information that comprises the steps:

analyzing a delocalized representation of a chemical structure, wherein at least a portion
of the delocalized structure representation describes a polycyclic ring system;
identifying, based on valence information, a plurality of fixed bond representation
candidates for at least a portion of the chemical structure;
evaluating at least a subset of the fixed bond representation candidates;
selecting from among the plurality of fixed bond representation candidates based on the
evaluation;
producing fixed bond information based on the selection; and
outputting the fixed bond information.

The delocalized representation of the chemical structure is analyzed and a plurality of fixed bond

representation candidates are identified. At least a subset of the candidates are evaluated, in part,

to allow selection of certain candidates. Next, fixed bond information is produced based on the

selection.

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First, Graovac is quite different from the invention defined by independent claim 5.

Graovac does not derive fixed bond representations from delocalized ones. Contrary to the

assertions made in the Office Action, the present disclosure provides numerous definitions and

reference to delocalized structure representations. See pages 23-24 and Fig. 21, for example.

Further, one skilled in the art would appreciate the differences between fixed and non-fixed bond

representations. Graovac is not concerned with deriving fixed bond information. In fact, there is

no disclosure or suggestion in the reference that could reasonably be interpreted as deriving fixed

bond information. Contrary to the claimed invention, Graovac is concerned with computing the

relative contribution (i.e., the Kekulé index) of a particular (given) fixed bond representation

with respect to the manifold of alternative valence bond depictions. Graovac's method is only

applicable to all-carbon systems. Graovac is not at all concerned with generating fixed-bond

representations from delocalized ones. As applied to claim 5, there is absolutely no disclosure or

suggestion in Graovac for the steps of:

> analyzing a delocalized representation of a chemical structure, wherein at least a portion
> of the delocalized structure representation describes a polycyclic ring system;
> identifying, based on valence information, a plurality of fixed bond representation
> candidates for at least a portion of the chemical structure;
> evaluating at least a subset of the fixed bond representation candidates;
> selecting from among the plurality of fixed bond representation candidates based on the
> evaluation;
> producing fixed bond information based on the selection; and
> outputting the fixed bond information.

It is therefore respectfully submitted that independent claim 5 is allowable over the art of

record.

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Claims 11 and 15 depend from independent claim 5 and are also believed allowable for at

least the reasons set forth above with respect to claim 5. In addition, these claims each introduce

novel elements that independently render them patentable over the art of record.

The Office Action identifies Table I as disclosing a priority index arrangement. This is

not the case, however. Table I is nothing more than a compilation of Kekulé indices. Table I of

Graovac illustrates, in part, certain values that have been selected as input for calculating the

Kekulé index for individual valence structures of several benzenoid polycyclic systems. See

page 6268, column 2. This compilation is sorted in a desired order. This is done to reveal a

correlation between the Kekulé index and a value computed by molecular orbital theory. There

is simply no disclosure in Graovac for priority queuing, as set forth in the present claims,

particularly with respect to Table I.

Independent claim 20 defines a system for use in deriving fixed bond information. The

system comprises:

> an analyzer analyzing a delocalized representation of a chemical structure, wherein at
> least a portion of the delocalized representation describes a polycyclic ring system;
> an identifier identifying, based on valence information, a plurality of fixed bond
> representation candidates for at least a portion of the chemical structure;
> an evaluator evaluating at least a subset of the fixed bond representation candidates;
> a selector electing from among the plurality of fixed bond representation candidates
> based on the evaluation;
> a producer producing fixed bond information based on the selection;
> said fixed bond information being output by the system.

The components of claim 20 can provide, at least in part, functions that are similar to the steps

recited in claim 5. As previously stated, Graovac does not disclose or suggest these features.

It is therefore respectfully submitted that independent claim 20 is allowable over the art

of record.

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For the reasons stated above, it is respectfully submitted that all of the pending claims (5-16 and 19-21) are now in condition for allowance. Therefore, a Notice of Allowance is believed in order, and courteously solicited.

The Examiner is respectfully requested to contact the undersigned, if it is believed that such contact would further the examination of the present application.

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AUTHORIZATION

The Commissioner is hereby authorized to charge any additional fees that may be

required for this Response, or credit any overpayment, to deposit account number 08-0219.

In the event that an extension of time is required, or which may be required in addition to

that requested in a petition for an extension of time, the Commissioner is requested to grant a

petition for that extension of which is required to make this response timely, and is hereby

authorized to charge any fee for such, to deposit account number 08-0219.

Respectfully submitted,

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28 Oct 2004

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